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Hard and Soft equivariance priors via Steerable CNNs

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Hard and Soft equivariance priors via Steerable CNNs

First, due credit to my amazing collaborators!

Maurice Weiler* and Gabriele Cesa*. General E(2)-Equivariant Steerable CNNs, Neural Information Processing Systems, 2019

Gabriele Cesa, Leon Lang, Maurice Weiler, A Program to build E(n)-Equivariant Steerable CNNs, International Conference on Representation Learning, 2022

Maksim Zhdanov, Nico Hoffmann, Gabriele Cesa, Implicit Convolutional Kernels for Steerable CNNs. Neural Information Processing Systems, 2023

Lars Veefkind and Gabriele Cesa. A Probabilistic Approach to Learning the Degree of Equivariance in Steerable CNNs. *International Conference* ₂ on Machine Learning. 2024

Agenda

From Group Convolution to Steerable Filters

Steerable Fields and Representation Theory

Steerable CNNs

Hard Priors: solving the exact kernel constraint

Soft Priors: learnable kernel constraint

Equivariance: CNN (rotation equivariance?)

Convolution: $(\mathbb{R}^n, +)$ - equivariance

Group Convolution: $(\mathbb{R}^n, +) \rtimes C_4$ - equivariance

Taco S. Cohen and Max Welling, Group Equivariant Convolutional Networks, International Conference on Machine Learning (ICML), 2016

Group Convolution (lifting convolution): $(\mathbb{R}^n, +) \rtimes C_4$ - equivariance

Taco S. Cohen and Max Welling, Group Equivariant Convolutional Networks, International Conference on Machine Learning (ICML), 2016

Group Convolution

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Group Convolution: Challenges

$$
[\kappa * f](g) = \int_{x \in X} \kappa(g^{-1} x) f(x) d\mu(x)
$$

- Often some form of discretization is required (potential artifacts!)
- What if input or output are not in $L^2(\mathbb{R}^n)$ or $L^2(G)$?
	- e.g. vector fields?
- The group G might be infinite or too large to fully enumerate
	- $G = SO(3)$ rotations of a point cloud
	- $n!$ permutations of a set or nodes of a graph

Group Convolution

 $L^2(\mathbb{Z}^2) \to L^2((\mathbb{Z}^2, +) \rtimes C_4)$

Isotropic Filters $\kappa \star \cdot$]: $L^2(\mathbb{Z}^2) \to L^2(\mathbb{Z}^2)$

• Isotropic filters: the response does not change when rotated

- Not very expressive
- Analogous to Graph Message Passing: no directional dependence!

• Filter can be rotated via linear combination

$$
[R_{\theta}. \kappa](r, \phi) = \kappa(r, \phi - \theta)
$$

= $w(r) \cos(\phi + \beta - \theta)$
= $w(r) \cos(\phi + \beta) \cos \theta - w(r) \sin(\phi + \beta) \sin \theta$
= $\cos \theta \kappa(r, \phi) - \sin \theta \kappa \left(r, \phi - \frac{\pi}{2}\right)$
= $\cos \theta \kappa(r, \phi) - \sin \theta R_{\frac{\pi}{2}} \kappa(r, \phi)$

 $= \cos \theta \cdot \cdot \cdot - \sin \theta \cdot \cdot$ $\kappa(r, \phi) = w(r) \cos(\phi + \beta)$ θ $r \mid \phi$

• e.g. filters used for edge-detection in classical Computer Vision

William T. Freeman and Edward H. Adelson. The design and use of steerable filters. IEEE Transactions on Pattern Analysis & Machine Intelligence, 1991

• Filter can be rotated via linear combination

Thanks to *linearity* of convolution operator:

$$
R_{\theta}. \kappa * f = \left(\cos \theta \kappa - \sin \theta \frac{R_{\pi}}{2} \kappa\right) * f
$$

$$
= \cos \theta \left(\kappa * f\right) - \sin \theta \left(\frac{R_{\pi}}{2} \kappa * f\right)
$$

• Filter can be rotated via linear combination

$$
R_{\theta} \cdot \kappa \star f = \cos \theta \left(\kappa \star f \right) - \sin \theta \left(R_{\frac{\pi}{2}} \cdot \kappa \star f \right)
$$

• Filter can be rotated via linear combination

 \star = θ

$$
R_{\theta} \cdot \kappa \star f = \cos \theta \left(\kappa \star f \right) - \sin \theta \left(R_{\frac{\pi}{2}} \cdot \kappa \star f \right)
$$

 $\rho(\theta)=$

 $\cos \theta$ – $\sin \theta$

 $\sin \theta$ $\cos \theta$

Steerable Filters: Other examples

• Filter can be rotated via linear combination

 $D^j(\alpha, \beta, \gamma) \in \mathbb{R}^{2j+1 \times 2j+1}$ Wigner D-matrix

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Feature Fields

- Interpret features as a multi-channels signal $f: \mathbb{R}^n \to \mathbb{R}^d$
- Signal transforms under (point) symmetry group G according to a transformation law
	- symmetry group G : e.g. rotations or reflections
	- N.B.: before we used G to also indicate translations
	- For now, we will implicitly consider equivariance to $(\mathbb{R}^n, +) \rtimes G$

$$
[\n\underset{\mathbb{C}}{\mathbb{X}}^{\mathbb{X}}\star \qquad]:\mathbb{R}^2 \to \mathbb{R}^1 \qquad [\n\underset{\mathbb{C}}{\mathbb{X}}^{\mathbb{X}}\star \qquad]:\mathbb{R}^2 \to \mathbb{R}^2
$$

Feature Fields and Steerable CNNs

- Interpret features as a multi-channels signal $f: \mathbb{R}^n \to \mathbb{R}^d$
- Signal transforms under (point) symmetry group G according to a transformation law
	- symmetry group $G : e.g.$ rotations or reflections
- Type of transformation identified by a representation of $G \to \mathbb{R}^d \times d$

$$
[g.f](x) = \rho(g)f(g^{-1}x)
$$

$$
[\n\mathbf{M}^* \star \mathbf{M}] : \mathbb{R}^2 \to \mathbb{R}^1 \qquad [\n\mathbf{M}^* \star \mathbf{M}] : \mathbb{R}^2 \to \mathbb{R}^2
$$

Feature Fields and Steerable CNNs

- Interpret features as a multi-channels signal $f: \mathbb{R}^n \to \mathbb{R}^d$
- Signal transforms under (point) symmetry group G according to a transformation law
	- symmetry group $G : e.g.$ rotations or reflections
- Type of transformation identified by a representation of $G \to \mathbb{R}^d \times d$

$$
f = \begin{bmatrix} 1 & \frac{1}{2} & \frac{1
$$

Definition: Representation of a Compact Group

A *(real) representation* $\rho: G \to GL(\mathbb{R}^d)$ of a *compact group* G is a map which associates to each element $q \in G$ an *invertible* $d \times d$ matrix s.t.:

- $\forall a, b \quad \rho(a)\rho(b) = \rho(ab)$
- $\forall a \ \rho(a)^{-1} = \rho(a^{-1})$
- $\rho(e) = \text{Id}_{d \times d}$

Definition: Representation of a Compact Group

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Can assume w.l.o.g. *orthogonal* representations, i.e. that $\rho(g)^{-1} = \rho(g)^T$

Describes the action of a group G on a *vector space* $V = \mathbb{R}^d$

E.g. representations of the rotation group $SO(2)$

• Trivial representation

 $\rho(r_{\rm A})=1$

• Standard representation

 $f(t,\cdot) \colon \mathcal{C}_4 \to \mathbb{R}$

0 0 1

 $\mathbf{0}$

 θ

Direct Sum

Formally: the Regular Representation

- \cdot $L^2(G)$ is the vector space of square integrable functions on G
- $L^2(G)$ carries an orthogonal action of G

 $g.f](x) \coloneqq f(g^{-1}x)$ $g: L^2(G) \to L^2(G)$, $f \mapsto g \cdot f$

• This is the *Regular Representation* of G

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- $L^2(G)$ carries an orthogonal action of G

 $g.f](x) \coloneqq f(g^{-1}x)$ $g: L^2(G) \to L^2(G)$, $f \mapsto g \cdot f$

- This is the *Regular Representation* of G
- When G is a finite group it looks like permutation matrices (e.g. C_4)

$$
\rho(r^0) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \rho(r^1) = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \rho(r^2) = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \rho(r^3) = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{bmatrix}
$$

One Theorem To Rule Them All: Peter-Weyl theorem

- Let G be a *compact* group
- There is a set of *irreducible representations (irreps)* denoted \widehat{G}
	- analogous to frequencies in classical Fourier Transform
	- e.g. circular harmonics or Wigner-D Matrices

The matrix coefficients of the *irreps* form an *orthogonal basis* for $L^2(G)$

$$
f(g) = \sum_{\psi \in \hat{G}} \sqrt{d_{\psi}} \sum_{1 \le i j \le d_{\psi}} \hat{f}(\psi)_{ij} \psi(g)_{ij}
$$

$$
\psi_0(\theta) = 1 \quad \psi_1(\theta) = \begin{bmatrix} \cos 1\theta & -\sin 1\theta \\ \sin 1\theta & \cos 1\theta \end{bmatrix} \quad \psi_2(\theta) = \begin{bmatrix} \cos 2\theta & -\sin 2\theta \\ \sin 2\theta & \cos 2\theta \end{bmatrix} \quad \psi_3(\theta) = \begin{bmatrix} \cos 3\theta & -\sin 3\theta \\ \sin 3\theta & \cos 3\theta \end{bmatrix}
$$

One Theorem To Rule Them All: Peter-Weyl theorem

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$$

 $\hat{f}(\psi) \in \mathbb{R}^{d_{\psi} \times d_{\psi}}$ Contains the weights

One Theorem To Rule Them All: Peter-Weyl theorem

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f(g) = \sum_{\psi \in \hat{G}} \sqrt{d_{\psi}} \sum_{1 \le i j \le d_{\psi}} \hat{f}(\psi)_{ij} \psi(g)_{ij}
$$

Caveat: this is actually a basis only in $\mathbb C$, but sometimes it has redundant entries in ℝ, e.g.

$$
\psi_1(\theta) = \begin{bmatrix} \cos 1\theta & -\sin 1\theta \\ \sin 1\theta & \cos 1\theta \end{bmatrix}
$$

One Theorem To Rule Them All: Peter-Weyl theorem (Pt. 2)

- Let G be a *compact* group
- There is a set of *irreducible representations (irreps)* denoted \hat{G}
	- analogous to frequencies in classical Fourier Transform
	- e.g. circular harmonics or Wigner-D Matrices

Any unitary representation ρ can be decomposed as a *direct sum* of *irreps* up to a change of basis Q_{ρ}

$$
\rho(g) = Q_{\rho}^{T} \left(\bigoplus_{\psi_{i} \in \hat{G}} \bigoplus_{r}^{[i(\rho)]} \psi_{i}(g) \right) Q_{\rho}
$$

$$
\rho(\theta) = \begin{bmatrix} 1 & & & \\ & \begin{bmatrix} \cos 1\theta & -\sin 1\theta \\ \sin 1\theta & \cos 1\theta \end{bmatrix} \\ & & \begin{bmatrix} \cos 2\theta & -\sin 2\theta \\ \sin 2\theta & \cos 2\theta \end{bmatrix} \end{bmatrix}
$$

What did we find?

- Group convolution with steerable filters produces smaller steerable features
	- No need to store redundant activations
- So far, only studied lifting convolution $L^2(\mathbb{R}^n) \to L^2((\mathbb{R}^n, +) \rtimes G)$
	- Input is a scalar field
	- Recover lifting convolution when using output regular representation
- What about other input fields? Intermediate layers?

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Feature Fields and Steerable CNNs

- Symmetry group G
- An intermediate feature is a multi-channels signal $f_l \colon \mathbb{R}^n \to \mathbb{R}^d$
- Associated with its own transformation law ρ_l
- Steerable CNN is equivariant when each layer Ψ_l commutes with its input and output transformations

Given a choice of input and output steerable feature types, what convolution do we need to use?

• What kind of filters produce an output feature map with the *desired transformation type*?

Steerable CNNs

• Standard *convolution* with G-steerable filter K guarantees also G equivariance

$$
K: \mathbb{R}^n \to \mathbb{R}^{d_{out} \times d_{in}} \longrightarrow
$$

$$
K(x) = \rho_{out}(g)K(g^{-1}, x)\rho_{in}(g)^T \longrightarrow
$$

Maurice Weiler, Mario Geiger, Max Welling, Wouter Boomsma and Taco Cohen, 3D Steerable CNNs: Learning Rotationally Equivariant Features in Volumetric Data, Conference on Neural Information Processing Systems (NIPS), 2018

Taco Cohen, Mario Geiger and Maurice Weiler, A General Theory of Equivariant CNNs on Homogeneous Spaces, Conference on Neural Information Processing Systems (NeurIPS), 2019

Steerable CNNs

• Standard *convolution* with G-steerable filter K guarantees also G equivariance

$$
K: \mathbb{R}^n \to \mathbb{R}^{d_{out} \times d_{in}} \longrightarrow K(x) = \rho_{out}(g)K(g^{-1}, x)\rho_{in}(g)^T \longrightarrow \text{Cov}_{\text{Sov}_{i}} \longrightarrow \text{Cov}_{\text{Sov}_{i
$$

 $Q:$ How do we parameterize G -steerable filters?

Equivariant Non-Linearities

- Let the intermediate feature $f: \mathbb{R}^n \to \mathbb{R}^d$ transform under $\rho: G \to O(d)$
- The quantity $|f(x)|_2^2 \in \mathbb{R}^+$ is invariant
	- norm non-linearity: $f(x) \mapsto \sigma(|f(x)|_2^2) f(x)$ (Worrall et al., 2017)
	- **gated non-linearity:** $f(x)$, $f_g(x) \mapsto \sigma(f_g(x)) f(x)$ (Weiler et al., 2018)
		- where $f_g(x)$ is another, invariant, feature field transforming under $\rho(g) = 1$
- Can also use other quadratic invariants:
	- tensor-product: $f(x) \mapsto f(x) \otimes f(x) \in \mathbb{R}^{d^2}$ (Kondor et al., 2018)
	- output transforms under $\rho_{out} = \rho \otimes \rho$
- $(x, y, z) \otimes (x, y, z) = vec$ x^2 xy xz xy y^2 yz xz yz z^2
- Fourier-based pointwise non-linearities (imitate GCNN)
	- feature vector $f(x) \in \mathbb{R}^d$ represents a bandlimited signal in $L^2(G)$
	- Compose: (discrete) Fourier Transform ∘ σ ∘ (discrete) Inverse Fourier Transform
	- Band-limit + sufficient samples to control *reconstruction error*

Daniel E. Worrall, Stephan J. Garbin, Daniyar Turmukhambetov, and Gabriel J. Brostow. Harmonic networks: Deep translation and rotation equivariance. Conference on Computer Vision and Pattern Recognition (CVPR), 2017. Maurice Weiler, Mario Geiger, Max Welling, Wouter Boomsma, and Taco S. Cohen. 3D steerable CNNs: Leaming rotationally equivariant features in volumetric data. Conference on Neural Information Processing Systems (NeurlPS), Risi Kondor, Zhen Lin, and Shubhendu Trivedi. Clebsch-gordan nets: a fully Fourier space spherical convolutional neural network. Advances in Neural Information Processing Systems (NeurIPS), 2018. Nadav Dym, and Haggai Maron. On the Universality of Rotation Equivariant Point Cloud Networks. International Conference on Learning Representations (ICML). 2020.

Outcome: equivariance to continuous rotations

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Soft Priors: learnable kernel constraint

Solving the steerability constraint

• Standard *convolution* with G-steerable filter K guarantees also G equivariance

$$
K: \mathbb{R}^n \to \mathbb{R}^{d_{out} \times d_{in}} \longrightarrow
$$

$$
K(x) = \rho_{out}(g)K(g^{-1}, x)\rho_{in}(g)^T \longrightarrow
$$

$$
K(x) = \rho_{out}(g)K(g^{-1}, x)\rho_{in}(g)^T
$$

 $Q:$ How do we parameterize G -steerable filters?

Solving the steerability constraint: Overall Strategy

- 1. Linear projection Π: space of *unconstrained kernels* → space of *equivariant kernels*
- 2. Pick a convenient basis for the **domain** of Π: space of *unconstrained kernels*
- 3. Project to find a basis for the image of Π: space of *equivariant kernels*

$$
K(x) = \rho_{out}(g)K(g^{-1}.x)\rho_{in}(g)^{T}
$$

Solving the steerability constraint: Projection

• Linear projection Π: space of *unconstrained kernels* \mapsto space of *equivariant kernels*

$$
K': \mathbb{R}^n \to \mathbb{R}^{d_{out} \times d_{in}} \qquad \qquad \longrightarrow \qquad K = \Pi[K'] \colon \mathbb{R}^n \to \mathbb{R}^{d_{out} \times d_{in}}
$$

$$
K(x) = \rho_{out}(g)K(g^{-1}.x)\rho_{in}(g)^{T}
$$

Solving the steerability constraint: Reynolds Operator

• Linear projection Π: space of *unconstrained kernels* \mapsto space of *equivariant kernels*

$$
K': \mathbb{R}^n \to \mathbb{R}^{d_{out} \times d_{in}} \qquad \qquad \longrightarrow \qquad K = \Pi[K'] : \mathbb{R}^n \to \mathbb{R}^{d_{out} \times d_{in}}
$$

$$
K(x) = \rho_{out}(g)K(g^{-1}.x)\rho_{in}(g)^{T}
$$

$$
\Pi[K'](x) = \int_{G} \rho_{out}(g)K'(g^{-1}.x)\rho_{in}(g)^{T} dg
$$

Solving the steerability constraint: Kernel Vectorization

- Consider the vectorized kernel $\kappa(x) = vec(K(x))$
	- Column-wise vectorization of the matrix $K(x)$

Identity $\frac{\nu_{ec}(ABC^T)}{K_{\text{FOPool}}} = \frac{C \otimes A_{\text{FPO}}}{K_{\text{FOPool}}}$ Kronecker product $A \otimes B = \begin{bmatrix} a_{11} & B & \cdots & a_{1n} & B \\ \vdots & \vdots & a_{1n} & B \\ a_{n1} & B & \cdots & a_{nn} & B \end{bmatrix}$ $\rho_{in} \otimes \rho_{out}: G \rightarrow \mathbb{R}(d_{out} \cdot d_{in}) \times (d_{out} \cdot d_{in})$

$$
\kappa(x) = [(\rho_{in} \otimes \rho_{out})(g)] \kappa(g^{-1}, x)
$$

 $\kappa \colon \mathbb{R}^n \to \mathbb{R}^{d_{out} \cdot d_{in}}$

$$
\Pi[\kappa'](x) = \int_G (\rho_{in} \otimes \rho_{out})(g) \kappa'(g^{-1}.x) dg
$$

Solving the steerability constraint: Steerable Basis

• Assume a G-steerable basis $B=\{Y_j^k:\mathbb R^n\to\mathbb R^{d_j}\mid\psi_j\in\widehat G,k\}$ for $L^2(\mathbb R^n)$ (Freeman & Adelson, 1991)

$$
Y_j^k(g^{-1}.x) = \psi_j(g)^T Y_j^k(x)
$$

ŵ $-\sin j\theta$ $\psi_j(\theta) = \begin{bmatrix} \cos \theta & \sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}$

Peter-Weyl Theorem B forms the change of basis

$$
\kappa'(x) = \sum_{j,k} W_{j,k} Y_j^k(x)
$$

$$
\kappa(x) = \Pi[\kappa'](x) = \int_G (\rho_{in} \otimes \rho_{out})(g) \kappa'(g^{-1}.x) dg
$$

=
$$
\int_G (\rho_{in} \otimes \rho_{out})(g) \sum_{j,k} W_{j,k} Y_j^k(g^{-1}.x) dg
$$

$$
\kappa(x) = \Pi[\kappa'](x) = \int_G (\rho_{in} \otimes \rho_{out})(g) \kappa'(g^{-1}.x) dg
$$

=
$$
\int_G (\rho_{in} \otimes \rho_{out})(g) \sum_{j,k} W_{j,k} \psi_j(g)^T Y_j^k(x) dg
$$

$$
\kappa(x) = \Pi[\kappa'](x) = \int_G (\rho_{in} \otimes \rho_{out})(g)\kappa'(g^{-1}.x) dg
$$

=
$$
\sum_{j,k} \left[\int_G (\rho_{in} \otimes \rho_{out})(g)W_{j,k} \psi_j(g)^T dg \right] Y_j^k(x)
$$

$$
\kappa(x) = \Pi[\kappa'](x) = \int_G (\rho_{in} \otimes \rho_{out})(g) \kappa'(g^{-1}.x) dg
$$

=
$$
\sum_{j,k} unvec[\sum_{j,k} \sum_{\psi_{e\in (Ag_{\mathcal{C}})} \in (c \otimes A) \cup e_{c(\beta)}} \prod_{j,k} \sum_{\psi_{e\in (Ag_{\mathcal{C}})} \in (c \otimes A) \cup e_{c(\beta)}} \prod_{j,k} (\psi_j \otimes \rho_{in} \otimes \rho_{out})(g) dg] vec(W_{j,k})
$$

Solving the steerability constraint: Assume Irreps

• W.I.o.g. assume input and output representations are *irreducible representations*

• That is
$$
\rho_{out} = \psi_J
$$
 and $\rho_{in} = \psi_l$

$$
\kappa(x) = \Pi[\kappa'](x) = \int_G (\psi_l \otimes \psi_j)(g) \kappa'(g^{-1}.x) dg
$$

=
$$
\sum_{j,k} unvec[\sqrt{\sum_{j,k}^k(x)}]
$$

$$
\left[\int_G (\psi_j \otimes \psi_l \otimes \psi_j)(g) dg \right] vec(W_{j,k}
$$

Solving the steerability constraint: Decompose Tensor Products

• Tensor products can be decomposed as a direct sum of irreps via Clebsh-Gordan transform

$$
\kappa(x) = \Pi[\kappa'](x) = \int_G (\psi_l \otimes \psi_j)(g) \kappa'(g^{-1}.x) dg
$$

=
$$
\sum_{j,k} unvec[\bigcup_{g} (\psi_j \otimes \psi_l \otimes \psi_j)(g) dg \bigg] vec(W_{j,k}
$$

Leon Lang and Maurice Weiler. A Wigner-Eckart theorem for group equivariant convolution kernels. International Conference on Learning Representations, 2020 Gabriele Cesa, Leon Lang, and Maurice Weiler. A program to build $E(N)$ -equivariant steerable CNNs. *International Conference on Learning Representations. 2021* Lars Veefkind and Gabriele Cesa. A Probabilistic Approach to Learning the Degree of Equivariance in Steerable CNNs. International Conference on Machine Learning. 2024 Peter-Weyl Theorem

Solving the steerability constraint: Decompose Tensor Products

• Tensor products can be decomposed as a direct sum of irreps via Clebsh-Gordan transform

$$
\kappa(x) = \Pi[\kappa'](x) = \int_G (\psi_l \otimes \psi_j)(g) \kappa'(g^{-1}.x) dg
$$

=
$$
\sum_{j,k} unvec[\bigcup_{g} Y_j^k(x)]
$$

$$
\int_G \varrho_{jlj}^T \left(\bigoplus_i \bigoplus_{r} \psi_i(g) \right) \varrho_{jlj} dg \bigg] vec(W_{j,k})
$$

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$$
\kappa(x) = \Pi[\kappa'](x) = \int_G (\psi_l \otimes \psi_j)(g) \kappa'(g^{-1}.x) dg
$$

=
$$
\sum_{j,k} unvec[\bigotimes_{j,l} Y_j^k(x)
$$

$$
Q_{jlj}^T \left(\bigoplus_i \bigoplus_{r}^{[i(j_l])]} \left[\int_G \psi_i(g) dg \right] \right) Q_{jlj} vec(W_{j,k})
$$

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Solving the steerability constraint: Recall Fourier Transform

• The matrix coefficients of the *irreducible representations* form an *orthogonal basis*

$$
\kappa(x) = \Pi[\kappa'](x) = \int_G (\psi_l \otimes \psi_j)(g) \kappa'(g^{-1}.x) dg
$$

=
$$
\sum_{j,k} \text{unvec}[\mathbf{y}_j^k(x)]
$$

$$
Q_{jij}^T \left(\bigoplus_i \bigoplus_j \left[\int_G \psi_i(g) \psi_0(g) dg \right] \right) Q_{jij} \text{vec}(W_{j,k})
$$

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• The matrix coefficients of the *irreducible representations* form an *orthogonal basis*

$$
\kappa(x) = \Pi[\kappa'](x) = \int_G (\psi_l \otimes \psi_j)(g) \kappa'(g^{-1}.x) dg
$$

=
$$
\sum_{j,k} unvec[\bigotimes_{j,l} Y_j^k(x)
$$

$$
Q_{jlj}^T \left(\bigoplus_{i} \bigoplus_{r}^{[i(j_l)]} \delta_{i=0} \right) Q_{jlj} vec(W_{j,k}
$$

Leon Lang and Maurice Weiler. A Wigner-Eckart theorem for group equivariant convolution kernels. International Conference on Learning Representations, 2020 Gabriele Cesa, Leon Lang, and Maurice Weiler. A program to build $E(N)$ -equivariant steerable CNNs. *International Conference on Learning Representations. 2021* Lars Veefkind and Gabriele Cesa. A Probabilistic Approach to Learning the Degree of Equivariance in Steerable CNNs. International Conference on Machine Learning. 2024 **Peter-Weyl Theorem**
orthogonality matrix coefficients
of the irreps

Solving the steerability constraint: Sparse Subset of Weights

• The matrix coefficients of the *irreducible representations* form an *orthogonal basis*

$$
\kappa(x) = \Pi[\kappa'](x) = \int_G (\psi_l \otimes \psi_j)(g) \kappa'(g^{-1}.x) dg
$$

=
$$
\sum_{j,k} unvec[\text{ }] Y_j^k(x)
$$

$$
\Pi_{jlj} = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}
$$

Leon Lang and Maurice Weiler. A Wigner-Eckart theorem for group equivariant convolution kernels. International Conference on Learning Representations, 2020 Gabriele Cesa, Leon Lang, and Maurice Weiler. A program to build $E(N)$ -equivariant steerable CNNs. *International Conference on Learning Representations. 2021* Lars Veefkind and Gabriele Cesa. A Probabilistic Approach to Learning the Degree of Equivariance in Steerable CNNs. International Conference on Machine Learning. 2024

Result

- Complete theoretical description of the space of -steerable filters
	- For any compact G and any transformation laws ρ_{in} , ρ_{out}
- Algorithm to explicitly construct the steerable convolution layers
- General implementation in the form of a PyTorch library:

github.com/QUVA-Lab/escnn

General Program to implement G -equivariance: 2D images

2D rotational symmetries

\mathbb{R}^2 , +) $\rtimes G$ < $E(2)$

Maurice Weiler* and Gabriele Cesa*. General E(2)-Equivariant Steerable CNNs, Neural Information Processing Systems (NeurIPS), 2019

MNIST Variations

General Program to implement G -equivariance: 3D voxel data

Axial rotational

symmetries in 3D

Table 2: ModelNet10 $(O(2)$ symmetry)

Gabriele Cesa, Leon Lang, Maurice Weiler,

A Program to build E(n)-Equivariant Steerable CNNs,

International Conference on Representation Learning, 2022

Beyond fixed Steerable Basis

ModelNet40 Axial rotational symmetries in 3D

Learn G -equivariant MLP to parameterize G -steerable kernel $\kappa_{\theta}(q, x) = [(\rho_{in} \otimes \rho_{out})(q)] \kappa_{\theta}(x)$

Local Symmetries: Symmetries vary between features and scales

- Reflection symmetry in the class
- Rotational symmetry in the *local* patterns

source: [MikeLynch,](https://commons.wikimedia.org/wiki/File:Sunflower_Field_near_Raichur,_India.jpg) CC BY-SA 3.0

source: [Tiffany Bailey,](https://commons.wikimedia.org/wiki/File:Gendo_the_Hedgehog_(6111053153).jpg) **[CC BY 2.0](https://creativecommons.org/licenses/by/2.0/legalcode)**

Maurice Weiler* and Gabriele Cesa*. General E(2)-Equivariant Steerable CNNs, Neural Information Processing Systems (NeurIPS), 2019

Group Restriction

- Model the loss of symmetries at larger scales by relaxing the equivariance constraint at different depths:
	- exploit more symmetries in the first layers
	- restrict later to the symmetries of your output

Maurice Weiler* and Gabriele Cesa*. General E(2)-Equivariant Steerable CNNs, Neural Information Processing Systems (NeurIPS), 2019

Experiments on Natural Images

AA = Auto Augment

STL -10

Maurice Weiler* and Gabriele Cesa*. General E(2)-Equivariant Steerable CNNs, Neural Information Processing Systems (NeurIPS), 2019

Imperfect or Unknown symmetries

- Group Restriction: layer adapted to the symmetries manifested in the scale of its field of view
	- Still requires knowledge about these symmetries
- Can we *learn* the level of equivariance from data?

Finzi, M., Benton, G., and Wilson, A. G. Residual pathway priors for soft equivariance constraints. Advances in Neural Information Processing Systems (NeurIPS) 2021. van der Ouderaa, T., Romero, D. W., and van der Wilk, M. Relaxing equivariance constraints with non-stationary continuous filters. Advances in Neural Information Processing Systems (NeurIPS), 2022

Wang, R., Walters, R., and Yu, R. Approximately equivariant networks for imperfectly symmetric dynamics. International Conference on Machine Learning (ICML), 2022 Romero, D. W. and Lohit, S. Learning partial equivariances from data. Advances in Neural Information Processing Systems (NeurIPS), 2022

Agenda

From Group Convolution to Steerable Filters

Steerable Fields and Representation Theory

Steerable CNNs

Hard Priors: solving the exact kernel constraint

Soft Priors: learnable kernel constraint

Learnable Soft Prior

Learn *probability distribution* λ over a large group G

- \cdot uniform: indicates equivariance over full group G
- Supported on subgroup $H \subset G$: indicates equivariance over full group G
- Low values outside subgroup $H \subset G$: indicates "soft / relaxed prior"

Learnable steerability constraint: Reynolds Operator

• Linear projection Π: space of *unconstrained kernels* \mapsto space of *equivariant kernels*

$$
K': \mathbb{R}^n \to \mathbb{R}^{d_{out} \times d_{in}} \qquad \qquad \longrightarrow \qquad K = \Pi[K'] : \mathbb{R}^n \to \mathbb{R}^{d_{out} \times d_{in}}
$$

$$
K(x) = \rho_{out}(g)K(g^{-1}.x)\rho_{in}(g)^{T}
$$

$$
\Pi[K'](x) = \int_{G} \rho_{out}(g)K'(g^{-1}.x)\rho_{in}(g)^{T} dg
$$

Learnable steerability constraint: Reynolds Operator

• Linear projection Π: space of *unconstrained kernels* \mapsto space of *equivariant kernels*

$$
K': \mathbb{R}^n \to \mathbb{R}^{d_{out} \times d_{in}} \qquad \qquad \longrightarrow \qquad K = \Pi_{\lambda}[K'] : \mathbb{R}^n \to \mathbb{R}^{d_{out} \times d_{in}}
$$

Learnable steerability constraint: Repeat Previous Derivations

$$
\kappa(x) = \Pi_{\lambda}[\kappa'](x) = \int_{G} (\psi_{l} \otimes \psi_{J})(g)\kappa'(g^{-1}.x)\lambda(g)dg
$$

=
$$
\sum_{j,k} unvec[\prod_{j} Y_{j}^{k}(x)
$$

$$
Q_{jlj}^{T} \left(\bigoplus_{i} \bigoplus_{r} \left[\int_{G} \psi_{i}(g)\lambda(g)dg\right]\right) Q_{jlj} vec(W_{j,k})
$$
Learnable steerability constraint: Recall Fourier Transform

• The matrix coefficients of the *irreducible representations* form an *orthogonal basis*

$$
\kappa(x) = \Pi_{\lambda}[\kappa'](x) = \int_{G} (\psi_{l} \otimes \psi_{J})(g)\kappa'(g^{-1}.x)\lambda(g)dg
$$

=
$$
\sum_{j,k} unvec[\lambda_{j}]\gamma_{j}^{k}(x)
$$

$$
Q_{jij}^{T}\left(\bigoplus_{i} \bigoplus_{r}^{[i(jl)]} [\int_{G} \psi_{i}(g)\lambda(g)dg]\right)Q_{jlj}vec(W_{j,k})
$$

Peter-Weyl Theorem

Learnable steerability constraint: Recall Fourier Transform

• The matrix coefficients of the *irreducible representations* form an *orthogonal basis*

$$
\kappa(x) = \Pi_{\lambda}[\kappa'](x) = \int_{G} (\psi_{l} \otimes \psi_{j})(g)\kappa'(g^{-1}.x)\lambda(g)dg
$$

$$
= \sum_{j,k} unvec[\lambda_{j}]\gamma_{j}^{k}(x)
$$

$$
Q_{jij}^{T}\left(\bigoplus_{i} \bigoplus_{r} \bigoplus_{\gamma=1}^{[i(jij)]} \frac{\hat{\lambda}(\psi_{i})}{\sqrt{d_{i}}}\right)Q_{jij} \text{ vec}(W_{j,k})
$$

Peter-Weyl Theorem

Learnable steerability constraint: Recall Fourier Transform

• The matrix coefficients of the *irreducible representations* form an *orthogonal basis*

$$
\kappa(x) = \Pi_{\lambda}[\kappa'](x) = \int_{G} (\psi_{l} \otimes \psi_{J})(g) \kappa'(g^{-1}.x) \lambda(g) dg
$$

$$
= \sum_{j,k} unvec[\prod_{\lambda j l J} Y_{j}^{k}(x)
$$

$$
P_{\lambda j l J} = \begin{bmatrix} \frac{\lambda(\psi_{1})}{\sqrt{d_{1}}} & \frac{\lambda(\psi_{2})}{\sqrt{d_{2}}} \\ \frac{\lambda(\psi_{3})}{\sqrt{d_{3}}} & \frac{\lambda(\psi_{4})}{\sqrt{d_{4}}} \end{bmatrix}
$$

Side to Side comparison

Side to Side comparison: Simple MLP Setting

 $\mathscr{U}_{k\left(\partial\right)}$ \geqslant $e^{i k \partial}$

Lars Veefkind and Gabriele Cesa. A Probabilistic Approach to Learning the Degree of Equivariance in Steerable CNNs. International Conference on Machine Learning. 2024

Learnable steerability constraint: Implementation Details

- Everything is *differentiable* : can directly backpropagate to $\hat{\lambda}(\psi_i)$
- Normalise λ to a PDF:

$$
\hat{\lambda} = FT\left(\text{softmax}\left(\text{IFT}(\hat{\lambda}')\right)\right)
$$

 $\hat{\lambda}^{\prime}$ is the Fourier Transform of the *log-likelihood* function

• Initialize λ to uniform distribution

$$
\hat{\lambda}(\psi_i) = \begin{cases} 1, & i = 0 \\ \mathbf{0}_{d_i \times d_i}, & i \neq 0 \end{cases}
$$

• *Tunable* band-limit L on $\hat{\lambda}$ to regularise the likelihood and reduce parameters:

Learnable steerability constraint: Implementation Details

• Regularize subsequent layers with KL-divergence:

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• Rectangular images containing 2 digits, independently transformed

(c) Local vs global 90 degree rotation.

(d) Local vs global 180 degree rotation.

 37

 $7\,$ 3

• Rectangular images containing 2 digits, independently transformed

 37

Maurice Weiler* and Gabriele Cesa*. General E(2)-Equivariant Steerable CNNs, Neural Information Processing Systems (NeurIPS), 2019 Finzi, M., Benton, G., and Wilson, A. G. Residual pathway priors for soft equivariance constraints. Advances in Neural Information Processing Systems (NeurIPS) 2021. Lars Veefkind and Gabriele Cesa. A Probabilistic Approach to Learning the Degree of Equivariance in Steerable CNNs. International Conference on Machine Learning. 2024

 $7\,$ 3

Evaluation on MedMNIST3D dataset

• 3D voxel data

Maurice Weiler* and Gabriele Cesa*. General E(2)-Equivariant Steerable CNNs, Neural Information Processing Systems (NeurIPS), 2019 Finzi, M., Benton, G., and Wilson, A. G. Residual pathway priors for soft equivariance constraints. Advances in Neural Information Processing Systems (NeurIPS) 2021. Lars Veefkind and Gabriele Cesa. A Probabilistic Approach to Learning the Degree of Equivariance in Steerable CNNs. International Conference on Machine Learning. 2024

Evaluation on Smoke and JetFlow simulations

• 2D frames from simulation

Maurice Weiler* and Gabriele Cesa*. General E(2)-Equivariant Steerable CNNs, Neural Information Processing Systems (NeurIPS), 2019 Finzi, M., Benton, G., and Wilson, A. G. Residual pathway priors for soft equivariance constraints. Advances in Neural Information Processing Systems (NeurIPS) 2021. Wang, R., Walters, R., and Yu, R. Approximately equivariant networks for imperfectly symmetric dynamics. International Conference on Machine Learning (ICML), 2022 Lars Veefkind and Gabriele Cesa. A Probabilistic Approach to Learning the Degree of Equivariance in Steerable CNNs. International Conference on Machine Learning. 2024

Conclusion

- Complete theoretical description of the space of -steerable filters
	- For any compact G and any transformation laws ρ_{in} , ρ_{out}
- Algorithm to explicitly construct the steerable convolution layers github.com/QUVA-Lab/escnn

- Effective way to relax hard inductive bias / learn it
	- Symmetries vary between features and scales.
	- Overconstraining leads to performance reductions.
	- CNN layers can be fine-tuned with group restrictions.

Maurice Weiler* and Gabriele Cesa*. General E(2)-Equivariant Steerable CNNs, Neural Information Processing Systems (NeurIPS), 2019 Gabriele Cesa, Leon Lang, Maurice Weiler, A Program to build E(n)-Equivariant Steerable CNNs, International Conference on Representation Learning, 2022 Maksim Zhdanov, Nico Hoffmann, Gabriele Cesa, Implicit Convolutional Kernels for Steerable CNNs. Neural Information Processing Systems, 2023 Lars Veefkind and Gabriele Cesa. A Probabilistic Approach to Learning the Degree of Equivariance in Steerable CNNs. International Conference on Machine Learning. 2024

Th a nk you

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Side to Side comparison: Simple MLP Setting

Lars Veefkind and Gabriele Cesa. A Probabilistic Approach to Learning the Degree of Equivariance in Steerable CNNs. International Conference on Machine Learning. 2024

Agenda

ILLUININGS

Other experiments

• Rectangular images containing 2 digits, independently transformed

 37

(b) $O(2)$ SCNN (a) CNN (c) Our $O(2)$ PSCNN

Figure 2. Confusion matrices for DDMNIST with $O(2)$ symmetries. Labelled 0-99 from top to bottom and left to right.

 $7\,$ 3

37 Effect of Band-Limiting on Double-MNIST

• Rectangular images containing 2 digits, independently transformed

Figure 4. Likelihoods and errors of the fifth $O(2)$ PSCNN layer trained on $SO(2)$ DDMNIST under various bandlimits L.

Table 21. Double MNIST test accuracies using various levels of bandlimiting for our $SO(2)$ and $O(2)$ P-SCNNs. For each symmetry, the highest accuracy is **bold**, and the highest for each network group within this type of symmetry is underlined. Standard deviations over 5 runs are denoted in parentheses.

 5.8

Effect of Bandlimiting on Smoke dataset

Table 23. Smoke RMSE scores and parameter counts (in millions, M) comparing $SO(2)$ equivariant RSteer with our $SO(2)$ -PSCNN using various levels of band-limiting. Note that a band-limit of $L = 6$ equates to performing no band-limiting at all. Standard deviations over 5 runs are denoted in parentheses.

Experiments with more effective architectures

Table 24. Test accuracies on OrganMNIST3D and DoubleMNIST comparing the performance of our baseline configurations (Gated) with the structurally non-invariant configurations using a Fourier based non-linearity. For each column, **bold** indicates the highest accuracy and underline denotes the highest accuracy for the given network group. Standard deviations over 5 runs are denoted in parentheses.

Agenda

MARITAGE

Groups

Group Conv

Non-Linearities

Running examples

Discrete planar translations: $(\mathbb{Z}^2, +)$

Discrete planar rotations: C_n

Symmetries of squared grid: $p4 = (\mathbb{Z}^2, +) \rtimes C_4$

 $p4 = (Z^2, +) \rtimes C_4$

Running examples

Discrete planar translations: $(\mathbb{Z}^2, +)$

Discrete planar rotations and mirroring : D_n

Symmetries of squared grid: $p4m = (\mathbb{Z}^2, +) \rtimes D_4$

 $p4m = (\mathbb{Z}^2, +) \rtimes D_4$

Generalize Convolution

Group cross-correlation:

Equivariant Non-Linearities

- Intermediate feature $f: \mathbb{R}^n \to \mathbb{R}^d$
- Transforms under representation of $G \mid \rho: G \to \mathbb{R}^{d \times d}$ $\qquad [g.f](x) = \rho(g)f(g^{-1}x)$
	-
- We can NOT always use point-wise non-linearities (e.g ReLU)

Equivariant Non-Linearities: Fourier Transform based

- Imitate a GCNN
- Choose a band-limited subset of irreps $\{\rho_i\}_{i\in I} \subset \hat{G}$
- A feature vector $f(x) \in \mathbb{R}^d$ represents a bandlimited signal in $L^2(G)$
- Apply point-wise non-linearity σ (e.g. ReLU) by:
	- Sampling the signal $f(x)$ on a finite subset $\mathcal{G} \subset \mathcal{G}$
	- Applying σ on each sample
	- Reconstruct a band-limited signal from the samples

Equivariant Non-Linearities: Fourier Transform based

- Imitate a GCNN
- Choose a band-limited subset of irreps $\{\rho_i\}_{i\in I} \subset \hat{G}$
- A feature vector $f(x) \in \mathbb{R}^d$ represents a bandlimited signal in $L^2(G)$
- Apply point-wise non-linearity σ (e.g. ReLU) by:
	- Sampling the signal $f(x)$ on a finite subset $G \subset G$ (discrete Inverse Fourier Transform)
	- Applying σ on each sample
	- **Reconstruct a band-limited signal from the samples** (discrete Fourier Transform)

• Band-limit + sufficient samples to control reconstruction error

Equivariant Non-Linearities: Fourier Transform based

- Imitate a GCNN
- Choose a band-limited subset of irreps $\{\rho_i\}_{i\in I} \subset \hat{G}$
- A feature vector $f(x) \in \mathbb{R}^d$ represents a bandlimited signal in $L^2(G)$
- Apply point-wise non-linearity σ (e.g. ReLU) by:
	- Sampling the signal $f(x)$ on a finite subset $\mathcal{G} \subset \mathcal{G}$ (discrete Inverse Fourier Transform)
	- Applying σ on each sample
	- Reconstruct a band-limited signal from the samples (discrete Fourier Transform)

• Can also consider functions on homogeneous space X rather than G for reduced complexity. Recall Spherical CNNs

Convolution and Message Passing

$$
[\kappa * f](y) = \sum_{x \in \mathbb{Z}^n} \kappa(x - y) f(x)
$$
Convolution and Message Passing

$$
[\kappa * f](y) = \sum_{x \in \mathbb{Z}^n} \kappa(x - y) f(x)
$$

$$
\kappa(x - y) f(x) \qquad [\kappa * f](i) = \sum_{j \in N_i} \kappa(x_i - x_j) f_j
$$

Nathaniel Thomas, Tess Smidt, Steven Kearnes, Lusann Yang, Li Li, Kai Kohlhoff, and Patrick Riley. Tensor field networks: Rotation-and translation-equivariant neural networks for 3d point clouds. (2018)